Supporting information for:

Synthesis and Characterization of Three-Coordinate Ni(III)-Imide Complexes

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1. Magnetization data

Figure 1. Magnetization as a function of temperature for [(dtbpe)Ni=NAd^{+}][B(Ar^{F})$_4^{-}$] (**3**)

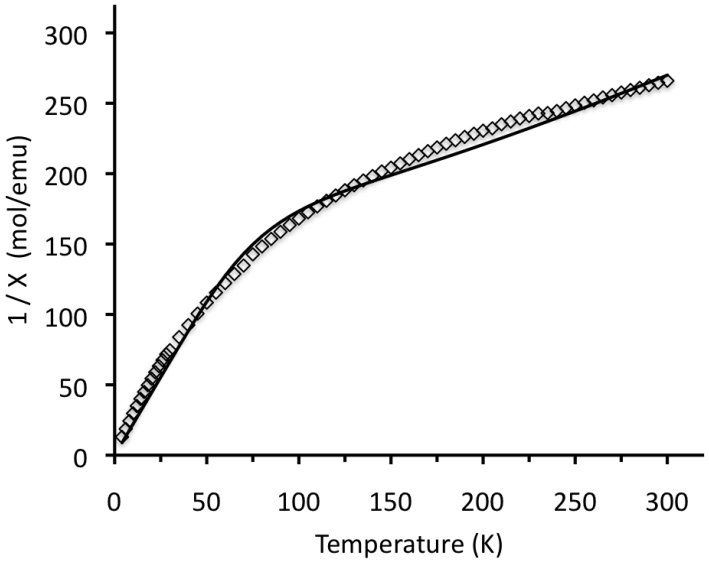


Figure 2. lnK vs 1/T for [(dtbpe)Ni=NAd^{+}][B(Ar^{F})$_4^{-}$] (**3**)

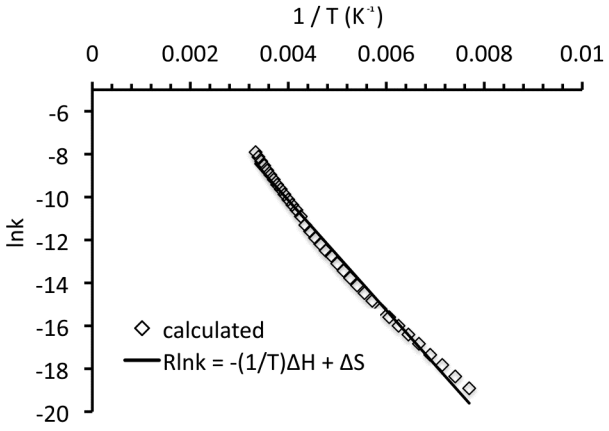


Figure 3. High-spin and low-spin molar fraction for [(dtbpe)Ni=NAd^{+}][B(Ar^{F})$_4^{-}$] (**3**)

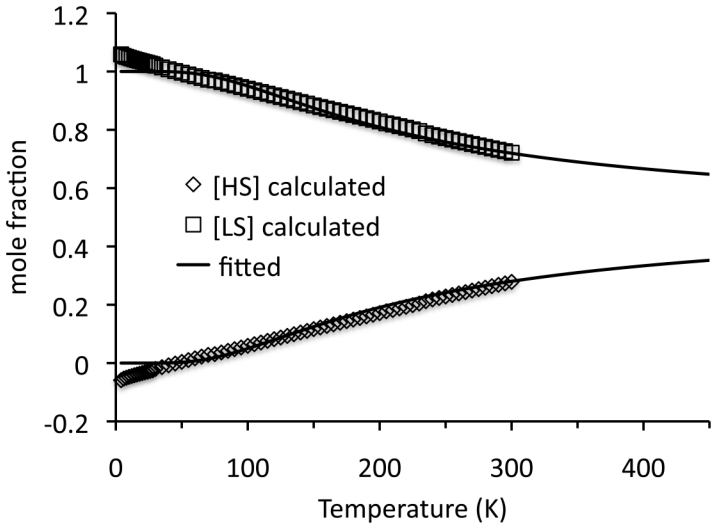
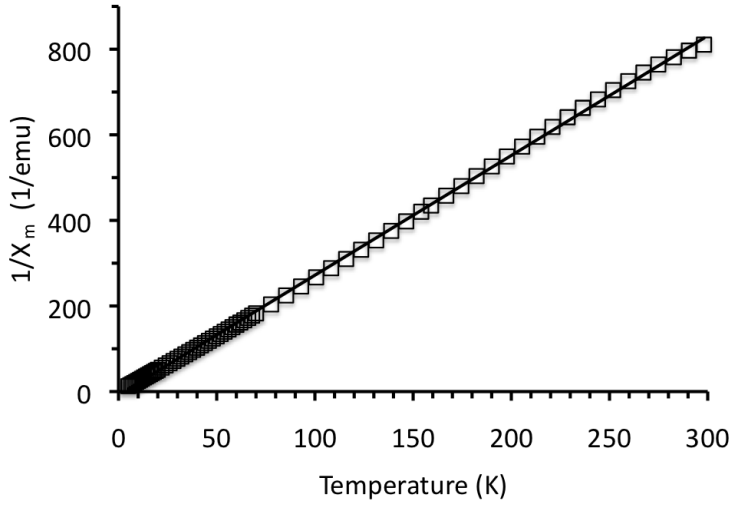


Figure 4. Solid-state magnetization for [(dtbpe)Ni=N(dmp)][B(Ar^{F})$_4^{-}$] (**8**)



2. EPR data

Figure 5. EPR data at different temperatures for [(dtbpe)Ni=NAd^{+}][B(Ar^{F})$_4^{-}$] (**3**)

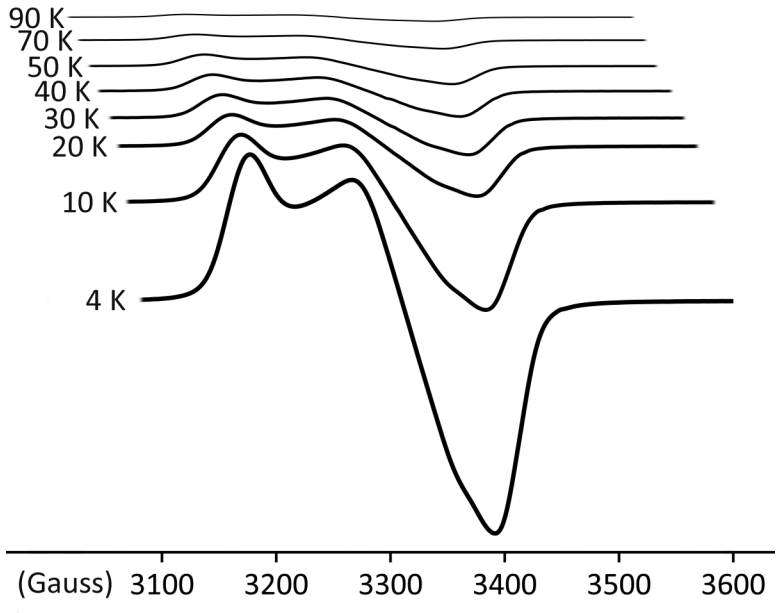


Figure 6. EPR data at different temperatures for [(dtbpe)Ni=N(dmp)$^{+}$][B(Ar^{F})$_4^{-}$] (**8**)

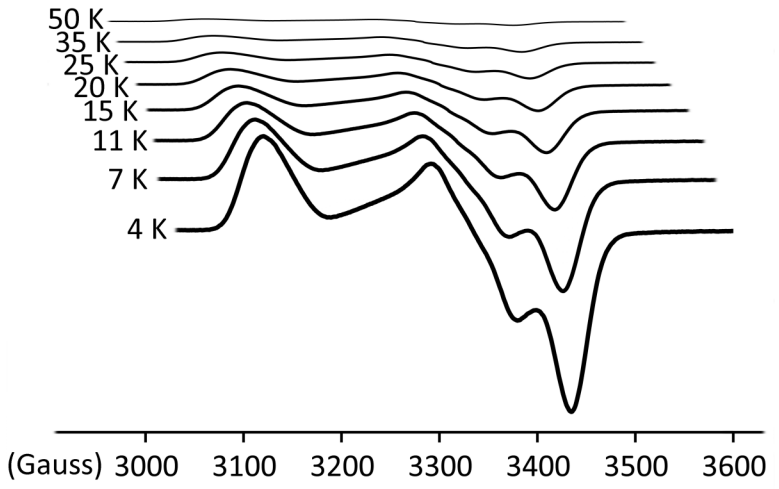


Table 1. Crystal data and structure refinement for [(dtbpe)Ni-N(H)Ad^{+}][B(Ar^{F})$_4^{-}$] (**2**).

Identification code	vlad115m	
Empirical formula	C_{60} H_{68} B F_{24} N Ni P_2	
Formula weight	1390.61	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P-1	
Unit cell dimensions	a = 16.6160(19) Å	α = 95.168(2)°.
	b = 19.441(2) Å	β = 100.073(2)°.
	c = 20.680(2) Å	γ = 103.594(2)°.
Volume	7474.1(17) Å^3	
Z	4	
Density (calculated)	1.459 Mg/m^3	
Absorption coefficient	0.466 mm^{-1}	
F(000)	2856	
Crystal size	0.05 x 0.03 x 0.02 mm^3	
Theta range for data collection	1.09 to 28.27°.	
Index ranges	$-22 \le h \le 20$, $-24 \le k \le 24$, $-26 \le l \le 27$	
Reflections collected	40000	
Independent reflections	28323 (R_{int} = 0.0514)	
Completeness to theta = 23.27°	90.2 %	
Absorption correction	Empirical	
Max. and min. transmission	0.3737 and 0.3152	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	28323 / 0 / 1611	
Goodness-of-fit on F^2	1.119	
Final R indices [I>2sigma(I)]	R1 = 0.0981, wR2 = 0.2048	
R indices (all data)	R1 = 0.1379, wR2 = 0.2238	
Largest diff. peak and hole	2.850 and -1.057 eÅ^{-3}	

Figure 7. Fully labeled ORTEP for [(dtbpe)Ni-N(H)Ad^{+}][B(Ar^{F})$_4^{-}$] (**2**)

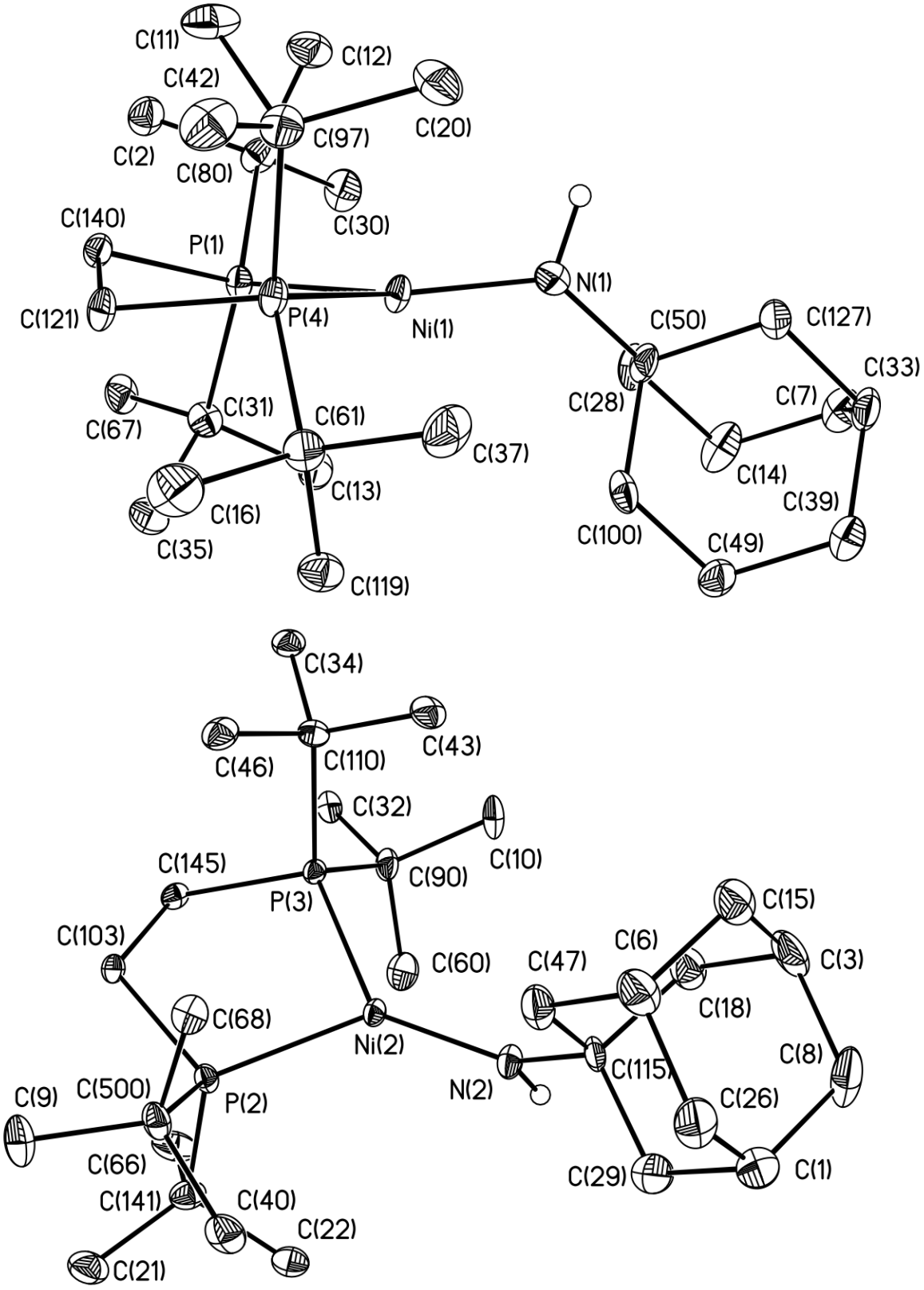


Table 2. Crystal data and structure refinement for [(dtbpe)Ni=NAd^{+}][B(Ar^{F})$_4^{-}$] (**3**).

Identification code	vlad111s	
Empirical formula	C_{60} H_{67} B F_{24} N Ni P_2	
Formula weight	1389.61	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	$P2_1/n$	
Unit cell dimensions	a = 17.736(5) Å	α = 90°.
	b = 16.476(4) Å	β = 112.082°.
	c = 23.481(6) Å	γ = 90°.
Volume	6358(3) Å^3	
Z	4	
Density (calculated)	1.452 Mg/m^3	
Absorption coefficient	0.465 mm^{-1}	
F(000)	2852	
Crystal size	0.6 x 0.5 x 0.3 mm^3	
Theta range for data collection	1.55 to 25.00°.	
Index ranges	$-16 \le h \le 21$, $-19 \le k \le 18$, $-27 \le l \le 27$	
Reflections collected	32564	
Independent reflections	11176 (R_{int} = 0.0381)	
Completeness to theta = 23.27°	99.9 %	
Absorption correction	Psi-scan	
Max. and min. transmission	0.9562 and 0.9315	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	11176 / 0 / 868	
Goodness-of-fit on F^2	1.236	
Final R indices [I>2sigma(I)]	R1 = 0.0717, wR2 = 0.1452	
R indices (all data)	R1 = 0.0837, wR2 = 0.1500	
Largest diff. peak and hole	0.685 and -0.351 eÅ^{-3}	

Figure 8. Fully labeled ORTEP for [(dtbpe)Ni=NAd^{+}][B(Ar^{F})$_4^{-}$] (**3**)

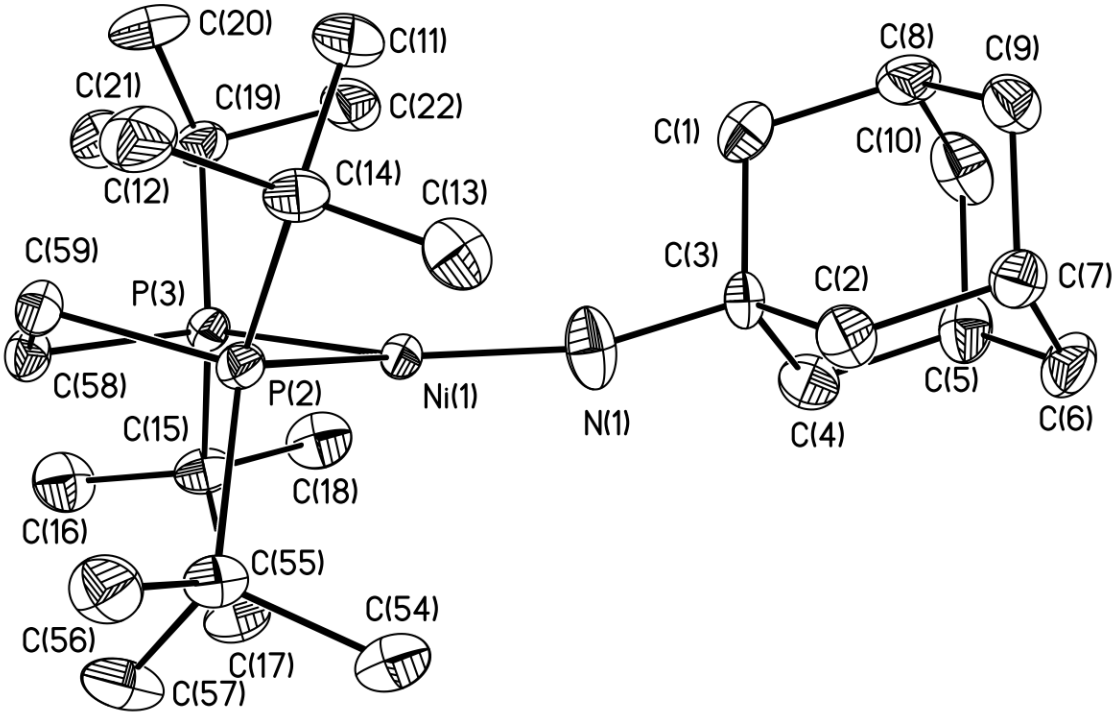
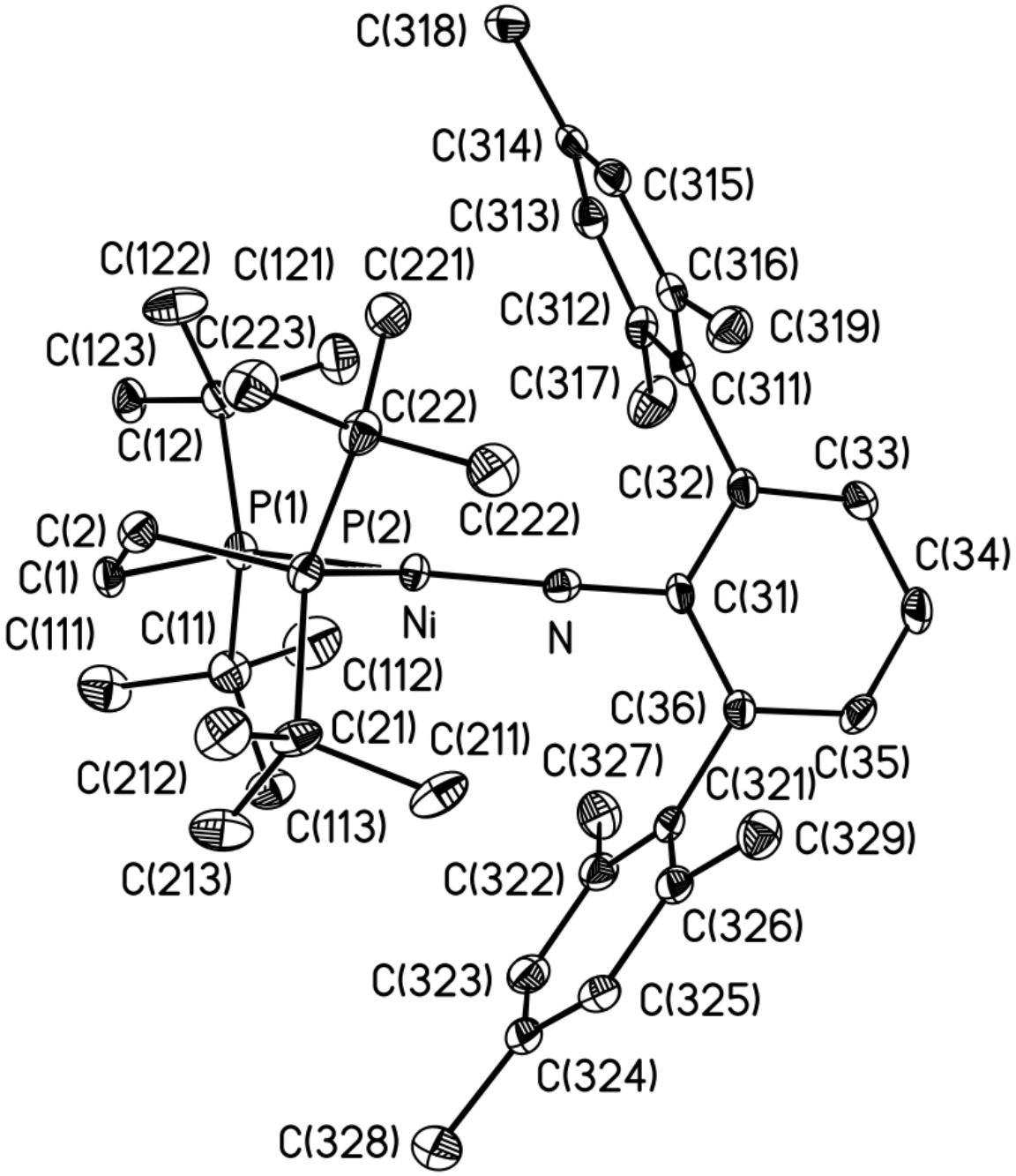


Table 3. Crystal data and structure refinement for [(dtbpe)Ni=N(dmp)$^{+}$][B(Ar^{F})$_4^{-}$] (**8**).

Identification code	vlad817m	
Empirical formula	C_{74} H_{77} B F_{24} N Ni P_2	
Formula weight	1567.83	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	$P2_1/n$	
Unit cell dimensions	a = 14.2589(12) Å	α = 90°.
	b = 113.0889(11) Å	β = 90.907°.
	c = 39.706(3) Å	γ = 90°.
Volume	7409.5(11) Å^3	
Z	4	
Density (calculated)	1.405 mg/m^3	
Absorption coefficient	0.408 mm^{-1}	
F(000)	3228	
Crystal size	0.06 x 0.05 x 0.05 mm^3	
Theta range for data collection	1.03 to 28.28°.	
Index ranges	$-18 \le h \le 18$, $-17 \le k \le 10$, $-49 \le l \le 52$	
Reflections collected	41170	
Independent reflections	16471 (R_{int} = 0.0774)	
Completeness to theta = 23.27°	99.1 %	
Absorption correction	Psi-scan	
Max. and min. transmission	0.977 and 0.960	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	16471 / 0 / 945	
Goodness-of-fit on F^2	0.972	
Final R indices [I>2sigma(I)]	R1 = 0.0714, wR2 = 0.1215	
R indices (all data)	R1 = 0.1241, wR2 = 0.1433	
Largest diff. peak and hole	0.775 and -0.439 eÅ^{-3}	

Figure 9. Fully labeled ORTEP for [([(dtbpe)Ni=N(dmp)$^{+}$][B(Ar^{F})$_4^{-}$] (**8**).



3. Computational details

Table 4. Calculated and measured metrical parameters.

	Crystal structure	Optimized (DFT)
[(dmpe)Ni=NC(CH_3)$_3^+$] (LS) model for: [(dtbpe)Ni=NAd$^+$] **(3)**	Ni–N = 1.657(5) Å P(2)–Ni = 2.1992(12) Å P(1)–Ni = 2.2041(12) Å N–C(3) = 1.424(7) Å P(2)–Ni–P(1) = 91.17(5)° P(2)–Ni–N = 132.28(13)° P(1)–Ni–N = 135.94(13)° Ni–N–C(3) = 165.2(4)°	1.821 Å 2.198 Å 2.202 Å 1.447 Å 1.112 Å 90.87° 132.24° 130.47° 153.89° 99.22° 106.91°
[(dmpe)Ni=NPh$^+$] (LS) model for: [(dtbpe)Ni=N(dmp)$^+$] **(8)**	Ni–N = 1.674(3) Å Ni–P(1) = 2.2314(11) Å Ni–P(2) = 2.2318(11) Å N–C(31) = 1.359(5) Å Ni–N–C(31) = 178.4(3)° P(1)–Ni–P(2) = 90.37(2)° P(1)–Ni–N = 133.81(10)° P(2)–Ni–N = 135.82(10)°	2.096 Å 2.259 Å 2.164 Å 2.112 Å 1.854 Å 1.542 Å 1.448 Å 106.74° 107.72° 106.94° 124.81° 39.56°

Table 5. Optimized geometry for (dmpe)Ni=NC(CH_3)$_3$.

No.	Atom	X	Y	Z
1	Ni	0.002490	0.007122	0.010487
2	P	0.022466	0.053728	2.342862
3	P	2.333619	-0.049798	0.060319
4	N	-1.224517	0.013300	-1.239850
5	C	1.838382	0.353215	2.844471
6	C	2.810331	-0.364853	1.880385
7	C	-0.437847	-1.567070	3.186527
8	C	-0.949691	1.353909	3.292647
9	C	3.291423	-1.345346	-0.910263
10	C	3.188533	1.571682	-0.376288
11	H	2.790199	2.387211	0.234888
12	H	3.002803	1.809739	-1.428132
13	H	4.268857	1.491978	-0.212969
14	H	2.905676	-2.343831	-0.683966
15	H	3.169969	-1.161913	-1.982221
16	H	4.357051	-1.303871	-0.660013
17	H	3.841253	-0.033618	2.053234
18	H	2.785135	-1.450607	2.038789
19	H	2.004485	1.437994	2.828330
20	H	1.995905	0.014259	3.875330
21	H	0.169357	-2.386776	2.790706
22	H	-0.284597	-1.493439	4.268752
23	H	-1.490064	-1.794229	2.989470
24	H	-0.715357	1.305224	4.361592
25	H	-2.021438	1.181535	3.154607
26	H	-0.708243	2.351883	2.914851
27	C	-2.232729	-0.000243	-2.273644
28	C	-2.600634	-1.482699	-2.587442
29	C	-3.479497	0.775944	-1.748391
30	C	-1.645680	0.699750	-3.537686
31	H	-4.253441	0.778490	-2.524442
32	H	-3.888590	0.296916	-0.851621
33	H	-3.222816	1.814363	-1.510269
34	H	-3.365295	-1.505752	-3.372506
35	H	-1.723846	-2.037510	-2.940463
36	H	-3.000576	-1.983639	-1.698466
37	H	-2.401997	0.701145	-4.330924
38	H	-1.370536	1.737617	-3.318390
39	H	-0.760234	0.167366	-3.903242

Table 6. Optimized geometry for (dmpe)Ni=NPh.

No	Atom	X	Y	Z
1	Ni	0.122676	-0.024909	-0.101435
2	P	-0.011540	0.029452	2.160512
3	P	2.381665	-0.069221	0.070829
4	C	2.819039	0.298617	1.899765
5	C	1.749103	-0.295008	2.844884
6	C	-0.497256	1.664985	2.976041
7	C	-1.068609	-1.212131	3.109315
8	C	3.262539	-1.709266	-0.261756
9	C	3.459623	1.155018	-0.876895
10	H	1.842176	0.119289	3.856903
11	H	2.859744	1.391147	2.002167
12	H	3.816416	-0.094025	2.135640
13	H	4.338845	-1.629961	-0.066396
14	H	3.391896	0.934145	-1.946978
15	H	3.101484	-1.992333	-1.306869
16	H	2.831657	-2.491750	0.370904
17	H	3.085883	2.170548	-0.713830
18	H	-0.446149	1.595576	4.069419
19	H	-1.517645	1.921968	2.674183
20	H	-0.899066	-1.136899	4.190197
21	H	0.169001	2.460411	2.627360
22	H	-0.832442	-2.225228	2.769505
23	H	-2.124317	-1.017563	2.894687
24	N	-0.985498	-0.024445	-1.375582
25	H	4.507635	1.092364	-0.559965
26	H	1.864297	-1.384404	2.920797
27	C	-1.873782	-0.023998	-2.401856
28	C	-1.478591	0.349799	-3.732028
29	C	-2.400927	0.325504	-4.786590
30	C	-3.752523	-0.022582	-4.571612
31	C	-4.158810	-0.371434	-3.264916
32	C	-3.247024	-0.397203	-2.201268
33	H	-3.562943	-0.691421	-1.202905
34	H	-5.196705	-0.643821	-3.076398
35	H	-4.464103	-0.022011	-5.393396
36	H	-2.065700	0.598356	-5.786661
37	H	-0.445085	0.643333	-3.901798

Table 7. Optimized geometry for [(dmpe)Ni=C$(CH_3)_3^+$] (low-spin isomer).

No.	Atom	X	Y	Z
1	Ni	-0.008557	0.013520	0.000415
2	P	0.011113	0.073684	2.326436
3	P	2.315858	-0.067138	0.048614
4	N	-1.197898	0.023902	-1.212565
5	C	1.829076	0.358365	2.828430
6	C	2.792535	-0.376241	1.869581
7	C	-0.466983	-1.537044	3.177715
8	C	-0.949512	1.391138	3.262235
9	C	3.254869	-1.379440	-0.916082
10	C	3.183989	1.543188	-0.399608
11	H	2.795746	2.366186	0.207901
12	H	2.997329	1.777035	-1.452122
13	H	4.263699	1.452168	-0.238551
14	H	2.857399	-2.371903	-0.684103
15	H	3.134423	-1.200419	-1.988775
16	H	4.320851	-1.348109	-0.665993
17	H	3.827097	-0.054967	2.039184
18	H	2.756202	-1.460654	2.034662
19	H	2.006139	1.441245	2.805152
20	H	1.982520	0.024941	3.861657
21	H	0.131870	-2.365558	2.787755
22	H	-0.313730	-1.456938	4.259424
23	H	-1.521196	-1.754309	2.980723
24	H	-0.717290	1.346639	4.331795
25	H	-2.022545	1.229168	3.122540
26	H	-0.696632	2.383580	2.877664
27	C	-2.202709	0.001829	-2.244900
28	C	-2.504781	-1.483380	-2.612008
29	C	-3.483911	0.701331	-1.693241
30	C	-1.650056	0.772996	-3.483181
31	H	-4.258197	0.696218	-2.469539
32	H	-3.868633	0.171132	-0.814777
33	H	-3.274282	1.740865	-1.417534
34	H	-3.271891	-1.514103	-3.394995
35	H	-1.604983	-1.983266	-2.988116
36	H	-2.876645	-2.033111	-1.739917
37	H	-2.405976	0.768141	-4.277347
38	H	-1.422790	1.813655	-3.225901
39	H	-0.741209	0.294832	-3.865570

Table 8. Optimized geometry for [(dmpe)Ni=C$(CH_3)_3^+$] (high-spin isomer).

No.	Atom	X	Y	Z
1	C	0.000000	0.000000	0.000000
2	P	0.000000	0.000000	1.883533
3	C	1.822836	0.000000	2.343394
4	Ni	-1.478219	-1.496518	2.878361
5	N	-1.531036	-3.175219	3.133570
6	C	-1.596039	-4.601582	3.326217
7	C	-2.308564	-4.880454	4.685629
8	P	-2.862665	0.305085	3.377625
9	C	-2.840500	0.859253	5.177656
10	C	-0.615181	1.740997	2.361562
11	C	-2.158644	1.791427	2.411267
12	C	-4.688249	0.270769	2.929760
13	C	-2.400855	-5.225879	2.145376
14	C	-0.138044	-5.157282	3.349866
15	H	-1.812619	1.036001	5.508330
16	H	-3.271947	0.074127	5.805942
17	H	-3.423740	1.778268	5.301103
18	H	-4.810988	0.006481	1.875309
19	H	-5.199299	-0.482360	3.537091
20	H	-5.145489	1.248928	3.114103
21	H	-2.500793	2.725776	2.871949
22	H	-2.583418	1.751312	1.400089
23	H	-0.185406	1.978618	3.343067
24	H	-0.226683	2.477704	1.648395
25	H	-1.018666	0.121875	-0.380257
26	H	0.628705	0.811910	-0.381483
27	H	0.389316	-0.955540	-0.364349
28	H	2.334059	0.851233	1.880879
29	H	2.287258	-0.927651	1.995650
30	H	1.935275	0.056815	3.430092
31	H	-0.170041	-6.242950	3.499816
32	H	0.371664	-4.951990	2.401776
33	H	0.438084	-4.709806	4.167442
34	H	-2.454286	-6.313057	2.278269
35	H	-3.422078	-4.829350	2.116272
36	H	-1.912652	-5.016903	1.186722
37	H	-2.362514	-5.963362	4.848535
38	H	-1.753838	-4.431035	5.516963
39	H	-3.328061	-4.478630	4.680246

Table 9. Optimized geometry for parallel [(dmpe)Ni=NPh$^+$] (low-spin isomer).

No	Atom	X	Y	Z
1	C	-0.007291	-0.000685	-0.004261
2	C	-0.010890	0.329055	1.373549
3	C	1.179691	0.355484	2.099662
4	C	2.427217	0.046100	1.443784
5	C	2.417169	-0.287582	0.039941
6	C	1.210722	-0.307155	-0.659717
7	N	3.582835	0.068168	2.131179
8	Ni	5.087511	0.096868	3.026328
9	P	5.717537	0.586348	5.201736
10	C	5.303164	-0.739887	6.473720
11	P	7.313035	-0.337793	2.549806
12	C	8.195227	0.997219	1.555812
13	C	8.222107	-0.368368	4.226028
14	C	7.622745	0.671476	5.199696
15	C	7.813273	-1.943597	1.708541
16	C	5.170971	2.191058	6.015825
17	H	5.666055	2.319023	6.984597
18	H	4.087618	2.172716	6.168865
19	H	5.414727	3.039711	5.369890
20	H	4.216479	-0.827776	6.567888
21	H	5.727618	-0.481608	7.450102
22	H	5.697851	-1.708606	6.152788
23	H	7.999847	0.513095	6.217016
24	H	7.901470	1.690393	4.902165
25	H	8.122773	-1.383804	4.630290
26	H	9.291137	-0.181972	4.068986
27	H	7.386175	-2.795652	2.245615
28	H	8.904085	-2.041015	1.683206
29	H	9.262757	0.767665	1.467059
30	H	7.757317	1.055501	0.554656
31	H	7.430623	-1.953741	0.683414
32	H	8.073898	1.971316	2.039139
33	H	1.191820	0.605920	3.156523
34	H	3.358483	-0.519791	-0.449782
35	H	-0.948594	0.562922	1.869802
36	H	1.206082	-0.559154	-1.716469
37	H	-0.940761	-0.018617	-0.559490

Table 10. Optimized geometry for parallel [(dippn)Ni=NPh^{+}] (high-spin isomer).

No	Atom	X	Y	Z
1	C	0.000000	0.000000	0.000000
2	C	0.000000	0.000000	1.412205
3	C	1.197323	0.000000	2.140046
4	C	2.466269	0.047026	1.467046
5	C	2.451062	0.069607	0.030160
6	C	1.240664	0.023690	-0.674210
7	N	3.632638	0.069209	2.160791
8	Ni	5.084008	0.096760	3.024083
9	P	5.692210	0.612820	5.145385
10	C	5.265758	-0.628150	6.506023
11	P	7.252337	-0.366017	2.554995
12	C	8.208854	0.883589	1.507745
13	C	8.208364	-0.366748	4.216334
14	C	7.607519	0.671163	5.191735
15	C	7.767026	-2.007224	1.778257
16	C	5.206447	2.253390	5.941801
17	H	5.704463	2.388822	6.909440
18	H	4.121632	2.272183	6.086862
19	H	5.475390	3.075524	5.271451
20	H	4.176736	-0.704265	6.587147
21	H	5.683267	-0.318566	7.471715
22	H	5.654767	-1.615470	6.237476
23	H	7.964942	0.504690	6.216058
24	H	7.900820	1.688393	4.899853
25	H	8.122037	-1.379814	4.631330
26	H	9.273687	-0.171778	4.038089
27	H	7.329915	-2.831717	2.349877
28	H	8.858457	-2.111988	1.756072
29	H	9.265033	0.602039	1.418692
30	H	7.758226	0.928843	0.511139
31	H	7.377520	-2.056060	0.756437
32	H	8.130745	1.877490	1.959750
33	H	1.188943	-0.026143	3.227402
34	H	3.401605	0.113702	-0.496739
35	H	-0.945831	-0.018532	1.952560
36	H	1.263778	0.024609	-1.763425
37	H	-0.934124	-0.017838	-0.555692

Table 11. Optimized geometry for perpendicular [(dmpe)Ni=NPh^{+}] (low-spin isomer).

No	Atom	X	Y	Z
1	Ni	0.000000	0.000000	0.000000
2	P	0.000000	0.000000	2.260154
3	P	2.260951	0.000000	0.031768
4	C	2.809808	0.313109	1.842982
5	C	1.803358	-0.314088	2.834607
6	C	3.179896	-1.594025	-0.414915
7	H	2.958561	-1.849829	-1.456191
8	H	2.820381	-2.411133	0.218876
9	H	4.263703	-1.479982	-0.288549
10	C	3.257626	1.291572	-0.921598
11	H	4.323346	1.246120	-0.665481
12	H	3.135395	1.114316	-1.995056
13	H	2.866042	2.287748	-0.693212
14	C	-0.464258	1.585790	3.184720
15	H	0.173325	2.407087	2.841889
16	H	-1.502572	1.841170	2.949411
17	H	-0.354582	1.463139	4.269394
18	C	-0.966367	-1.301024	3.231442
19	H	-0.729889	-2.293602	2.835619
20	H	-0.727179	-1.263354	4.301400
21	H	-2.038079	-1.124852	3.093461
22	H	1.948847	0.079768	3.848962
23	H	1.935557	-1.403355	2.879498
24	H	3.821688	-0.081592	2.002951
25	H	2.853578	1.402305	1.976259
26	N	-1.199687	-0.026429	-1.202745
27	C	-2.176345	-0.024735	-2.170509
28	C	-2.719799	1.199329	-2.682151
29	C	-3.715044	1.198175	-3.671076
30	C	-4.200789	-0.023175	-4.187926
31	C	-3.682789	-1.245265	-3.705408
32	C	-2.689979	-1.247898	-2.713993
33	H	-2.329519	2.128205	-2.272301
34	H	-4.114071	2.139809	-4.043974
35	H	-4.971635	-0.022561	-4.955943
36	H	-4.057346	-2.186286	-4.104325
37	H	-2.278371	-2.177341	-2.326968

Table 12. Optimized geometry for perpendicular [(dippn)Ni=NPh^{+}] (high-spin isomer).

No	Atom	X	Y	Z
1	C	-0.149931	-0.002007	-0.087533
2	C	0.194027	-1.094445	0.751025
3	C	1.386520	-1.087360	1.469616
4	C	2.290138	0.043094	1.362873
5	C	1.921614	1.149987	0.499845
6	C	0.720928	1.112867	-0.204030
7	N	3.438189	0.064285	2.045310
8	Ni	5.053134	0.094065	3.005019
9	P	5.772887	0.864035	5.166506
10	C	5.317323	-0.232064	6.633368
11	P	7.318498	-0.615540	2.619889
12	C	8.358303	0.492369	1.500935
13	C	8.169193	-0.468713	4.321846
14	C	7.678117	0.771967	5.105085
15	C	7.760692	-2.355226	2.048633
16	C	5.430568	2.605792	5.796923
17	H	5.982026	2.797028	6.723984
18	H	4.359479	2.720790	5.989835
19	H	5.727135	3.341252	5.042939
20	H	4.235189	-0.195492	6.793270
21	H	5.824286	0.109634	7.542487
22	H	5.598806	-1.270465	6.432697
23	H	8.076164	0.760349	6.127102
24	H	8.031631	1.695973	4.629200
25	H	7.946525	-1.390122	4.875602
26	H	9.256594	-0.427418	4.184179
27	H	7.261145	-3.094843	2.681688
28	H	8.843691	-2.513808	2.094314
29	H	9.408760	0.181737	1.518795
30	H	7.984438	0.426947	0.474355
31	H	7.423319	-2.498194	1.017415
32	H	8.285431	1.534866	1.825998
33	H	1.663826	-1.914965	2.116037
34	H	2.599155	1.995207	0.420929
35	H	-0.479514	-1.942864	0.832643
36	H	0.447848	1.943783	-0.848344
37	H	-1.083650	-0.019265	-0.642547

4. Complete reference 39

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